REMARKS

With respect to the microfiche appendix, the Office Action states that the copy of the postcard submitted does not appear to have been stamped indicated receipt of the materials. Submitted herewith is a copy of the original filing postcard indicated such receipt.

As amended, the claims are directed to deriving chemical structural information. A chemical name is preprocessed to produce a preprocessed name. While the preprocessed name is parsed into fragments, a parallel list of data objects is derived wherein each data object corresponds to a fragment. From the list of data objects, a data object is removed that corresponds to descriptive text that does not contribute information regarding chemical structure. From the list of data objects, a connection table is derived and a consolidated list of data objects is derived that contains fewer data objects that the list of data objects. The connection table is adjusted based on whether the consolidated list of data objects includes a stereochemical indicator. A representation of a chemical structure is derived from the connection table.

Claims 1-23 have been rejected under 35 U.S.C. 112 as containing new matter and as being unenabled. Claims 1-23 have been cancelled and new claims 24-44 have been added. Support for the new claims may be found in the specification at least where indicated below:

Claim 24: figs. 3A-3B and page 5, lines 13-15; page 13, line 14 through page 17, line 12; page 19, lines 3-12; page 19, line 19 through page 24, line 1; page 24, lines 2-8; page 24, lines 13-15.

Claim 25: page 6, line 3 through page 13, line 13.

Claim 26: page 13, lines 19-21.

Claim 27: page 17, lines 11-13.

Claim 28: page 19, line 9.

Claim 29: page 20, lines 4-10.

Claim 30: page 7, lines 2-4.

Claim 31: page 7, lines 9-11.

Claim 32: page 8, lines 6-7.

Claim 33: page 8, lines 15-18.

Claim 34: page 13, lines 14-19.

Claim 35: page 14, lines 16-18.

Claim 36: page 15, lines 4-5.

Claim 37: page 15, lines 10-12.

Claim 38: page 15, lines 13-14.

Claims 39-41: page 23, lines 15-17.

Claim 42: page 24, line 14.

Claim 43: page 24, lines 15-18.

Claim 44: figs. 3A-3B and page 5, lines 13-15; page 13, line 14 through page 17, line 12; page 19, lines 3-12; page 19, line 19 through page 24, line 1; page 24, lines 2-8; page 24, lines 13-15; page 28, line 12 through page 29, line 16; source code listing in microfiche appendix.

The Office Action's claim rejections relied on U.S. Patent No. 5,345,516 to Boyer et al. ("Boyer"). Boyer discloses an apparatus and method for optical recognition of chemical graphics that allows documents containing chemical structures to be optically scanned so that both the text and the chemical structures are recognized. The structures are converted directly into molecular structure files suitable for direct input into chemical databases, molecular modeling programs, image rendering programs and programs that perform real time manipulation of structures.

All of the pending claims 24-44 require, among other things, that a data object is removed that corresponds to descriptive text that does not contribute information regarding chemical structure, and that the connection table is adjusted based on whether the consolidated list of data objects includes a stereochemical indicator. Boyer neither discloses nor suggests removing a data object that corresponds to descriptive text that does not contribute information regarding chemical structure. Further, Boyer neither discloses nor suggests adjusting a connection table based on whether a consolidated list of data objects includes a stereochemical indicator. In fact, Boyer makes no mention at all of any stereochemical indicator. For at least these reasons, claims 24-44 are allowable over Boyer.

The applicant submits that the application is in condition for allowance, which action is requested.

The Commissioner is hereby authorized to charge any fee deficiency, or credit any overpayment to our Deposit Account No. 08-0219.

Respectfully submitted,

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Replacement Pages for Claims 1-44
(MARKED TO SHOW CHANGES)

[1. A method for use in deriving chemical structural information, comprising:

acquiring a chemical name lacking an association with a chemically accurate computer readable diagrammatic representation of a substance identified by the chemical name;

parsing the chemical name into at least first and second fragments, the first and second fragments having had non-contiguous positions in the chemical name; and

applying computer executable logic to the first and second fragments, the computer executable logic determining, based at least in part on the positions of the first and second fragments within the chemical name, respective first and second chemically accurate computer readable diagrammatic representations of the first and second fragments.

2. The method of claim 1, further comprising:

identifying, among a preselected set of text strings, respective first and second text strings that correspond to the first and second fragments; and

basing the determination of the first and second diagrammatic representations at least in part on conditions associated with the first and second text strings.

3. A system for use in deriving chemical structural information, comprising:

an acquiror acquiring a chemical name lacking an association with a chemically accurate computer readable diagrammatic representation of a substance identified by the chemical name;

a parser parsing the chemical name into at least first and second fragments, the first and second fragments having had non-contiguous positions in the chemical name; and

computer executable logic determining, based at least in part on the positions of the first and second fragments within the chemical name, respective first and second chemically accurate computer readable diagrammatic representations of the first and second fragments.

4. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive chemical structural information, the instructions causing the system to:

acquire a chemical name lacking an association with a chemically accurate computer readable diagrammatic representation of a substance identified by the chemical name;

parse the chemical name into at least first and second fragments, the first and second fragments having had non-contiguous positions in the chemical name; and

apply computer executable logic to the first and second fragments, the computer executable logic determining, based at least in part on the positions of the first and second fragments within the chemical name, respective first and second chemically accurate computer readable diagrammatic representations of the first and second fragments.

5. The method of claim 1, further comprising:

making a change to the chemical name to facilitate subsequent analysis of the chemical name.

6. The method of claim 1, further comprising:

detecting that the chemical name has an inverted form; and

changing the chemical name to an uninverted form.

7. The method of claim 1, further comprising:

inserting a delimiter into the chemical name.

8. The method of claim 1, further comprising:

comparing at least one of the first and second fragments to at least a portion of the contents of a set of chemical characteristics data.

9. The method of claim 8, further comprising:

associating at least one of the first and second fragments with a data object belonging to the set of chemical characteristics data.

10. The method of claim 9, wherein the data object includes a connection table.

11. The method of claim 9, wherein the data object includes a locant map.

12. The method of claim 9, wherein the data object includes an attach-in map.

13. The method of claim 9, wherein the data object includes an attach-out map.

14. The method of claim 8, further comprising:

selecting the portion of the contents as being representative of at least one of the first and second fragments; and

rejecting the portion of the contents in favor of another portion of the contents.

15. The method of claim 9, further comprising:

deriving at least one of the first and second chemically accurate computer readable diagrammatic representations from information belonging to the data object.

16. The computer software of claim 4, further comprising instructions for use in a computer system to help cause the computer system to:

make a change to the chemical name to facilitate subsequent analysis of the chemical name.

17. The computer software of claim 4, further comprising instructions for use in a computer system to help cause the computer system to:

detect that the chemical name has an inverted form; and

change the chemical name to an uninverted form.

18. The computer software of claim 4, further comprising instructions for use in a computer system to help cause the computer system to:

insert a delimiter into the chemical name.

19. The computer software of claim 4, further comprising instructions for use in a computer system to help cause the computer system to:

compare at least one of the first and second fragments to at least a portion of the contents of a set of chemical characteristics data.

20. The computer software of claim 19, further comprising instructions for use in a computer system to help cause the computer system to:

associate at least one of the first and second fragments with a data object belonging to the set of chemical characteristics data.

21. A method for use in deriving chemical structural information, comprising:

based on a processing rule, deriving first and second name fragments from a chemical name that lacks an association with a chemically accurate computer readable diagrammatic representation of a substance identified by the chemical name, the first and second fragments having non-contiguous positions in the chemical name;

determining type and position information for the first and second name fragments, the position information being descriptive of the positions of the first and second fragments within the chemical name;

based on a connectivity table and the first and second name fragments and the type and position information, determining at least a portion of a chemically accurate computer readable diagrammatic representation for the chemical name.

22. A system for use in deriving chemical structural information, comprising:

a derivor deriving, based on a processing rule, first and second name fragments from a chemical name that lacks an association with a chemically accurate computer readable

diagrammatic representation of a substance identified by the chemical name, the first and second fragments having non-contiguous positions in the chemical name;

a determiner determining type and position information for the first and second name fragments, the position information being descriptive of the positions of the first and second fragments within the chemical name;

a diagram determiner determining, based on a connectivity table and the first and second name fragments and the type and position information, at least a portion of a chemically accurate computer readable diagrammatic representation for the chemical name.

23. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive chemical structural information, the instructions causing the system to:

based on a processing rule, derive first and second name fragments from a chemical name that lacks an association with a chemically accurate computer readable diagrammatic representation of a substance identified by the chemical name, the first and second fragments having non-contiguous positions in the chemical name;

determine type and position information for the first and second name fragments, the position information being descriptive of the positions of the first and second fragments within the chemical name;

based on a connectivity table and the first and second name fragments and the type and position information, determine at least a portion of a chemically accurate computer readable diagrammatic representation for the chemical name.]

24. A method for use in deriving chemical structural information, the method comprising:

preprocessing a chemical name to produce a preprocessed name;

while parsing the preprocessed name into fragments, deriving a parallel list of data objects wherein each data object corresponds to a fragment;

removing from the list of data objects a data object that corresponds to descriptive text that does not contribute information regarding chemical structure;

deriving, from the list of data objects, a connection table and a consolidated list of data objects that contains fewer data objects that the list of data objects;

adjusting the connection table based on whether the consolidated list of data objects includes a stereochemical indicator; and

deriving a representation of a chemical structure from the connection table.

25. The method of claim 24, further comprising:

during preprocessing, converting at least a portion of the chemical name to an uninverted form.

26. The method of claim 24, further comprising:

during parsing, determining whether a match for a fragment is found in a dictionary of known text strings.

27. The method of claim 24, further comprising:

during derivation of the parallel list, choosing a data object having a highest rank.

28. The method of claim 24, further comprising:

during removal, determining that a data object corresponds to text including "solution".

29. The method of claim 24, further comprising:

during derivation of the consolidated list, determining whether a data object is misidentified.

30. The method of claim 24, further comprising:

counting parentheses in the chemical name.

31. The method of claim 24, further comprising:

in the chemical name, converting a hyphen to another character.

32. The method of claim 24, further comprising:

determining whether the chemical name includes the substring "mer".

33. The method of claim 24, further comprising:

determining whether the chemical name includes a character "2" that is not preceded by the character "d".

34. The method of claim 24, further comprising:

parsing "pentane" into fragments "pent" and "ane".

35. The method of claim 24, further comprising:

maintaining a repeat count for a data object.

36. The method of claim 24, further comprising:

further analyzing the consolidated list of data objects based on an association of individual atoms with respective specific locations in the connection table.

37. The method of claim 24, further comprising:

further analyzing the consolidated list of data objects based on a list of atoms identified in the connection table that are considered to be awaiting attachment.

38. The method of claim 24, further comprising:

further analyzing the consolidated list of data objects based on an association of a specific bond order to an attachment.

39. The method of claim 24, further comprising:

during derivation of the consolidated list of data objects, causing the consolidated list to reflect joining ligands to root structures.

40. The method of claim 24, further comprising:

during derivation of the consolidated list of data objects, causing the consolidated list to reflect joining cations to anions.

41. The method of claim 24, further comprising:

during derivation of the consolidated list of data objects, causing the consolidated list to reflect joining esters to acids.

42. The method of claim 24, further comprising:

deriving an image of the chemical structure.

43. The method of claim 24, further comprising:

determining whether the chemical name is uninterpretable.

44. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive chemical structural information, the instructions causing the system to:

preprocess a chemical name to produce a preprocessed name;

while parsing the preprocessed name into fragments, derive a parallel list of data objects wherein each data object corresponds to a fragment;

remove from the list of data objects a data object that corresponds to descriptive text that does not contribute information regarding chemical structure;

derive, from the list of data objects, a connection table and a consolidated list of data objects that contains fewer data objects that the list of data objects;

adjust the connection table based on whether the consolidated list of data objects includes a stereochemical indicator; and

derive a representation of a chemical structure from the connection table.

Replacement Pages for Claims 24-44

(CLEAN FORM)

24. A method for use in deriving chemical structural information, the method comprising:

preprocessing a chemical name to produce a preprocessed name;

while parsing the preprocessed name into fragments, deriving a parallel list of data objects wherein each data object corresponds to a fragment;

removing from the list of data objects a data object that corresponds to descriptive text that does not contribute information regarding chemical structure;

deriving, from the list of data objects, a connection table and a consolidated list of data objects that contains fewer data objects that the list of data objects;

adjusting the connection table based on whether the consolidated list of data objects includes a stereochemical indicator; and

deriving a representation of a chemical structure from the connection table.

25. The method of claim 24, further comprising:

during preprocessing, converting at least a portion of the chemical name to an uninverted form.

26. The method of claim 24, further comprising:

during parsing, determining whether a match for a fragment is found in a dictionary of known text strings.

27. The method of claim 24, further comprising:

during derivation of the parallel list, choosing a data object having a highest rank.

28. The method of claim 24, further comprising:

during removal, determining that a data object corresponds to text including "solution".

29. The method of claim 24, further comprising:

during derivation of the consolidated list, determining whether a data object is misidentified.

30. The method of claim 24, further comprising:

counting parentheses in the chemical name.

31. The method of claim 24, further comprising:

in the chemical name, converting a hyphen to another character.

32. The method of claim 24, further comprising:

determining whether the chemical name includes the substring "mer".

33. The method of claim 24, further comprising:

determining whether the chemical name includes a character "2" that is not preceded by the character "d".

34. The method of claim 24, further comprising:

parsing "pentane" into fragments "pent" and "ane".

35. The method of claim 24, further comprising:

maintaining a repeat count for a data object.

36. The method of claim 24, further comprising:

further analyzing the consolidated list of data objects based on an association of individual atoms with respective specific locations in the connection table.

37. The method of claim 24, further comprising:

further analyzing the consolidated list of data objects based on a list of atoms identified in the connection table that are considered to be awaiting attachment.

38. The method of claim 24, further comprising:

further analyzing the consolidated list of data objects based on an association of a specific bond order to an attachment.

39. The method of claim 24, further comprising:

during derivation of the consolidated list of data objects, causing the consolidated list to reflect joining ligands to root structures.

40. The method of claim 24, further comprising:

during derivation of the consolidated list of data objects, causing the consolidated list to reflect joining cations to anions.

41. The method of claim 24, further comprising:

during derivation of the consolidated list of data objects, causing the consolidated list to reflect joining esters to acids.

42. The method of claim 24, further comprising:

deriving an image of the chemical structure.

43. The method of claim 24, further comprising:

determining whether the chemical name is uninterpretable.

44. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive chemical structural information, the instructions causing the system to:

preprocess a chemical name to produce a preprocessed name;

while parsing the preprocessed name into fragments, derive a parallel list of data objects wherein each data object corresponds to a fragment;

remove from the list of data objects a data object that corresponds to descriptive text that does not contribute information regarding chemical structure;

derive, from the list of data objects, a connection table and a consolidated list of data objects that contains fewer data objects that the list of data objects;

adjust the connection table based on whether the consolidated list of data objects includes a stereochemical indicator; and

derive a representation of a chemical structure from the connection table.

Title: DERIVING CHEMICAL STRUCTURAL INFORMATION

Serial No: TBA Applicant Jonathan S. Brecher

In the above matter, the following have been received by the US Patent and Trademark Office on the date stamped hereon:

- ☒ Express Mail Label No. EM259723548US
- ☒ Application incl. 50 pages (___ Design)
  - 30 pp. of specification
  - 2 pp. of claims (# of claims - 1-6)
  - 1 pp. of abstract
  - 17 sheets of drawings; Figs. 1-7
  - ☐ formal ☒ informal
- ☐ Provisional Application Cover Sheet
- ☒ Declaration / Power of Attorney (X Unsigned)
- ☐ Verified Statement Claiming Small Entity Status
- ☐ Copy of Notice to File Missing Parts
- ☐ Request for filing CPA; 37 CFR 53(d)
- ☐ IDS; PTO-1449, and ___ references (Supp. ___)
- ☐ Certificate of Mailing under 37 CFR 1.8(a)
- ☐ Response to Office Action/Restriction Req.
- ☐ Petition for ___ month extension of time
- ☐ Assignment and Cover Sheet
- ☐ Amendment (☐ Preliminary; ☐ After Final)
- ☐ Notice of Appeal
- ☐ Appellant's Brief (triplicate) (☐ Reply Brief)
- ☐ Letter to Chief Draftsperson
- ☐ Issue Fee / ☐ Maintenance Fee Transmittal
- ☐ Sequence listing; ☐ Diskette
- ☒ Transmittal Letter
- ☐ Check for $_____; check # _____
- ☐ Deposit Account Authorization $ _____
- ☒ other: Appendix:NOMTOKENS and Cover Sheet for Appendix:NOMTOKENS
- ☒ other: Microfiche Appendix

Mailing Date: 02/11/00 Docket No. 10354/127 Atty/paralegal/secy: JAR:rh